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铁苋菜中的一个新化合物

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摘要 从云南省富民县产铁苋菜(*Acalypha australis* L.)全草中分离并鉴定了一个新化合物，命名为铁苋菜素(australisin)。通过光谱分析测定了其结构。此外，还分离到 β-谷甾醇(β-sitosterol)和胡萝卜甙(daucosterol)。

关键词 铁苋菜, 大戟科, 铁苋菜素

A NEW COMPOUND FROM ACALYPHA AUSTRALIS

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Abstract A new compound named australisin (1) was isolated from the whole herb of *Acalypha australis* L. (Euphorbiaceae). Its structure was established by a spectroscopic analysis. In addition, β-sitosterol and daucosterol were also obtained.

Key words *Acalypha australis*, Euphorbiaceae, Australisin

INTRODUCTION

Acalypha australis L. (Euphorbiaceae), annual herb, usually occours as a troublesome weed in farmlands and road sides throughout the southern China. The whole herb is used in the treatment of dysentery, diarrhea, abdominal distension, expectorant, uterus hemorrhage, dermatitis, and eczema [1,2]. Earlier work on the genus *Acalypha* showed the presences of alkaloid, amide, glucoside and sterol. [3,4]

We studied the chemical constituents of the whole herb of *Acalypha australis* L. collected in Fuming County, Yunnan Province, China in September, 1990. A new compound was isolated and named australisin (1). Its structure was determined by spectroscopic analysis.

RESULTS AND DISCUSSION

Australisin (1) showed the presences of three methoxy groups($CH_3O \times 3$), three methine groups (C-3,4,7), five quarternary carbons(C-5,6,8,9,10), two olefinic carbons(C-1′, C-2′) and four ketonic carbons(C-1,-COO- × 3) in the ^1H NMR and ^{13}C NMR(DEPT) spectra of (1) (Table 1). The IR absorptions were indicated of the presences of benzene ring(1600—1518cm^{-1}), hydroxl(3400cm^{-1}), and olefinic group(1615 cm^{-1}). The ^1H-^{13}C COSY spectrum of (1) showed the correlation signal between the C-2′(δ 129.7) and H-2′(δ 7.12), C-7 (δ 108.9) and H-7 (δ 7.88), C-4 (δ 35.6) and H-4(δ 6.21), C-3

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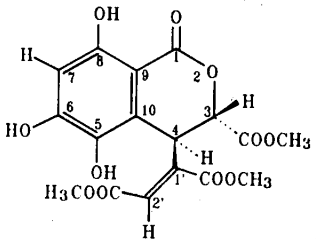
(δ79.4) and H-3(δ 5.88) and three correlation signals between the carbon and the hydrogen in each carboxymethyl group, respectively. In the $^1H-^1H$ COSY spectrum of (1), the coupling correlation signal between H-3 (δ 5.88) and H-4 (δ 6.21) with a small coupling constant (J = 1.6 Hz), H-4 (δ 6.21) and H-2′ (δ 7.12)could be observed, and the connection of C-3 and C-4 was determined. Therefore, we suggested that australisin possessed a carbon skeleton similar to chebulic acid (2) [5].

Table 1 ^1H NMR and ^{13}C NMR data of australisin(1)

(400 MHz, C_5D_5N, TMS)

C	δ_C(ppm)	δ_H(ppm)	C	δ_C(ppm)	δ_H(ppm)
1	164.7s		1′	143.3s	
3	79.4d	5.88(1H,d,J = 1.6Hz)	2′	129.7d	7.12(1H, br s)
4	35.6d	6.21(1H,br s)	$COOCH_3$	170.7s	
5	117.8s			52.9q	3.50(3H, s)
6	141.5s			166.9s	
7	108.9d	7.88(1H, s)		52.5q	3.50(3H, s)
8	147.6s			166.0s	
9	116.5s			52.1q	3.65(3H, s)
10	145.3s				

Assigments were based on $^1H-^{13}C$ COSY.



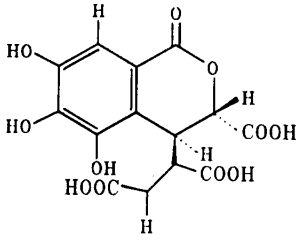


Fig.1: australisin(1) chebulic acid(2)

In order to determining the location of the aromatic proton, the COLOC spectrum of (1) was measured. It was the long-range correlation signals of (1) from its COLOC spectrum in Table 2. Therefore,the aromatic proton was located at the C-7 position.

Table 2 Long-range correlation signals from COLOC of australisin

(C_5D_5N, 400 MHz, TMS)

H	C-1	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-1′	C-2′	-COO- (166.0)	-COO- (166.9)	-COO- (170.7)
3	*		*					*		*				*
4		*		*				*	*	*	*		*	*
7	*			*	*		*	*						
2′			*							*			*	
$-OCH_3$ (3.65)												*		
$-OCH_3$ (3.50)													*	
$-OCH_3$ (3.50)														*

The unusual lowfield chemical shift for H-4(δ 6.21) was caused by two weak hydrogen bonding effection between $COOCH_3$-3 and H-4, and $COOCH_3$-1′ and H-4 (Fig. 2).

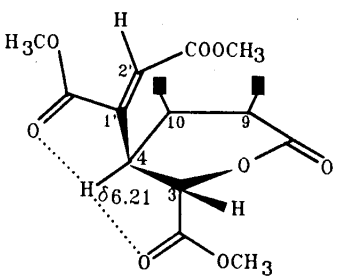


Fig.2: Hydrogen bonds within australisin(1)

Long-range coupling pattern between H-4 and H-2′ was observed in the ^1H-^1H COSY spectrum of (1), and the configuration of the double bond was a trans one. Thus, the structure of australisin is (1).

EXPERIMENTAL SECTION

Mps: uncorr.; IR: KBr; ^1H NMR (400.13MHz) and ^{13}C NMR (100.52 MHz), TMS as int. standard; EI-MS: 70eV.

Extraction and isolation: The air-dried whole plant (1300g) were powderd and extracted with MeOH (50℃). Evapn. of the solvent afford a residue (118g), which was descoloured by active charcoal and dissolved in H_2O. The aq. solution was extracted with EtOAc. The lipophilic phase (34g) was chromatographed over silica gel, eluted with the increasing proportions of PE-EtOAc. In the PE-EtOAc (3:7) eluation, australisin (0.05g) was obtained and finally purified by recrystalization.

Australisin(1), $C_{17}H_{16}O_{11}$, ([M]$^+$m / z396), colorless crystal. mp: 151— 153.5℃. IR ν_{max}^{KBr} cm^{-1}: 3400, 2950, 1725, 1615, 1600, 1518, 1485, 1430, 1375, 1300— 1225, 1110, 1050. EIMS m / z (70eV): 396 [M]$^+$, 305 (base). ^1H NMR and ^{13}C NMR data see Table 1.

β-Sitosterol, colorless needles. mp 140℃. $IR_{max}^{KBr}cm^{-1}$: 3500, 2930, 1470, 1380, 1065, 960. MS m / z:414, 396, 381, 329, 303, 273, 255, 213, 43.Mp, IR, TLC were identical with an authentic sample.

Daucosterol, amorphous powder. mp > 300℃. $IR_{max}^{KBr}cm^{-1}$:3400, 2960, 2930, 2850, 1450, 1375, 1360, 1160, 1100, 1075, 1025. IR and TLC were identical with an authentic sample.

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